

KINETICS OF FAST ATOMS IN THE TERRESTRIAL ATMOSPHERE

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Kinetics of Fast Atoms in the Terrestrial Atmosphere

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Final Report

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Introduction

This report summarizes our investigations performed under NASA Grant NAG5-8058. The three-year research supported by the Geospace Sciences SR&T program (Ionospheric, Thermospheric, and Mesospheric Physics) has been designed to investigate fluxes of energetic oxygen and nitrogen atoms in the terrestrial thermosphere. Fast atoms are produced due to absorption of the solar radiation and due to coupling between the ionosphere and the neutral thermospheric gas. We have investigated the impact of hot oxygen and nitrogen atoms on the thermal balance, chemistry and radiation properties of the terrestrial thermosphere. Our calculations have been focused on the accurate quantitative description of the thermalization of O and N energetic atoms in collisions with atom and molecules of the ambient neutral gas. Upward fluxes of oxygen and nitrogen atoms, the rate of atmospheric heating by hot oxygen atoms, and the energy input into translational and rotational-vibrational degrees of atmospheric molecules have been evaluated. Altitude profiles of hot oxygen and nitrogen atoms have been analyzed and compared with available observational data.

Energetic oxygen atoms in the terrestrial atmosphere have been investigated for decades, but insufficient information on the kinetics of fast atmospheric atoms has been a main obstacle for the interpretation of observational data and modeling of the hot geocorona. The recent development of accurate computational methods of the collisional kinetics is seen as an important step in the quantitative description of hot atoms in the thermosphere. Modeling of relaxation processes in the terrestrial atmosphere has incorporated data of recent observations, and theoretical predictions have been tested by new laboratory measurements.

The main results obtained under the present proposal are:

1. The method of numerical solution of the kinetic equation, describing thermalization process, has been developed and has been used to compute non-Maxwellian distributions of atmospheric oxygen and nitrogen atoms. Fluxes of hot O and N atoms in the terrestrial thermosphere have been obtained in numerical solutions of the time-dependent Boltzmann equation.

2. The rates of energy-transfer collisions of energetic O and N atoms with ambient gas have been computed with accurate collisional cross sections. The angular and energy dependences of cross sections were obtained in quantum calculations.

3. Thermalization times for energetic $O(^3P)$, $O(^1D)$, and $N(^4S)$ atoms and the atmospheric heating rate have been calculated at different altitudes for daytime and nighttime atmospheric conditions.

4. Fractions of energetic oxygen $O(^3P)$ atoms have been computed for altitudes of 200-700 km at different solar conditions, and theoretical results have been compared with observations.

5. Non-Maxwellian distributions of fast $N(^4S)$ atoms in the terrestrial atmosphere have been calculated with updated sources of nascent energetic nitrogen atoms. Computed distribution functions have been used for analysis of NO production rate in the terrestrial thermosphere. Theoretical results have been compared with observations.

6. Parameters of the upward flux of energetic $O(^3P)$ atoms have been determined in numerical calculations. The angular, energy, and altitude distributions of fast atoms in the upward flux near the exobase have been obtained from results of the Monte Carlo simulations of $O(^3P)+O(^3P)$ collisions carried out with realistic energy and angular dependent cross sections.

7. The probabilities of escape from the thermosphere to the exosphere have been computed for ground state $O(^3P)$ atoms produced at different altitudes below the exobase.

The description of the theoretical methods and obtained results have been published in our articles and reported on AGU Meetings:

Kharchenko V. and A. Dalgarno, *Fluxes of fast atoms near the terrestrial thermosphere*, Eos. Trans. AGU, **82**(20), S293 (2001)

Kharchenko V., A. Dalgarno, B. Zygelman, and J.-H. Yee, *Energy transfer in collisions of oxygen atoms in the terrestrial atmosphere*, J. Geophys. Res., **105**, 24899 (2000)

Kharchenko V., N. Balakrishnan, and A. Dalgarno, *The upward flux of fast oxygen atoms in the terrestrial thermosphere*, Eos. Trans. AGU, **81**, S333 (2000)

Balakrishnan N., E. Sergueeva, V. Kharchenko, and A. Dalgarno, *Kinetics and thermalization of hot $N(^4S)$ atoms in the upper atmosphere*, J. Geophys. Res., **105**, 18549 (2000)

Kharchenko V., and A. Dalgarno, *Fraction of energetic oxygen atoms in the upper terrestrial thermosphere*, Eos. Trans. AGU, **81**, F931 (2000)

Balakrishnan N., V. Kharchenko, and A. Dalgarno, *Translational energy relaxation of hot $O(^1D)$ atoms*, J. Phys. Chem., **103**, 3999 (1999)

Balakrishnan N., V. Kharchenko, and A. Dalgarno, *Translational energy relaxation of hot $O(^1D)$ atoms in collisions with N_2* , Eos. Trans. AGU, **80**, S239 (1999)

Results of our recent investigations of near exobase fluxes of energetic oxygen atoms and details of Monte Carlo simulations will be reported in

Kharchenko V. and A. Dalgarno, *Fast $O(^3P)$ and $O(^1D)$ atoms in the upper terrestrial thermosphere*, J. Geophys. Res., to be submitted (2002).

Differential and total cross sections for collisions of O and N atoms with the atmospheric gas

Nascent energetic atoms in the terrestrial thermosphere are produced by various photo-chemical and ionic reactions, and atmospheric sources of hot O and N have been carefully studied [Cotton *et al.* 1993; Gerard *et al.* 1995; Richards *et al.* 1994; Hickey *et al.* 1995; Shematovich *et al.* 1992, 1994; Fox and A. Hać, 1997]. Translational energies of nascent fast atoms are larger on two - three orders than thermal energy of the ambient gas, and hot atoms slow down in multiple collisions with thermal atmospheric atoms and molecules - O, N₂, and O₂. Energy distributions of fast O and N atoms, the rate of the atmospheric heating by fast atoms, and the energy input into translational and rotational-vibrational degrees of the bath gas molecules depend strongly on collisional cross sections. Calculations of these cross sections are complicated due to quantal character of atom -atom and atom-molecule collisions at eV's energies. Strong energy and angular dependences of realistic cross sections have to be taken into account in any evaluations of thermalization rates.

Accurate calculations of cross sections

Cross sections and thermalization rates for O + N₂, N and N + N₂, O₂ collisions have been obtained in our earlier calculations [Kharchenko *et al.* 1997, 1998; Balakrishnan *et al.* 1998a, 1998b]. Atom - molecule collisions are important in the low thermosphere, but collisions with atmospheric atomic oxygen dominate at altitudes above ~ 200 km. We performed accurate calculations of the energy transfer rate in O(³P) + O(³P) collisions [Zygelman, Kharchenko, and Dalgarno 1999; Kharchenko *et al.* 2000], which are the main thermalization mechanism in the middle and upper thermosphere. Cross sections for the thermalization of fast metastable O(¹D) atoms were also calculated [Balakrishnan *et al.* 1999] and compared with available experimental data [Matsumi *et al.* 1994, Matsumi and Chowdhury 1996].

We computed differential and total cross sections for elastic collisions of ground state oxygen atoms, using 18 electronic energy curves of O₂ molecules [Zygelman *et al.* 1994a,b]. Electronic states connected to the ground state of oxygen atoms are represented by singlet, triplet and quintet spin states. In Fig.1 the computed cross

sections for the individual spin states of colliding oxygen atoms are shown as functions of the kinetic energy.

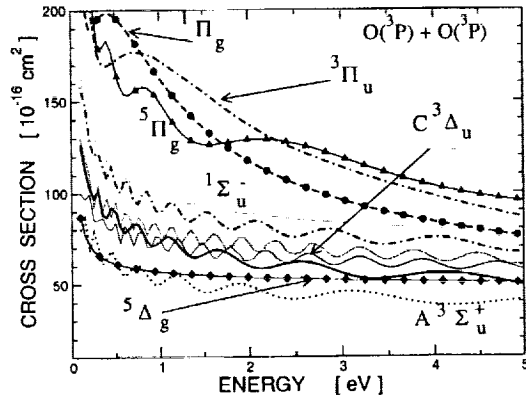


Fig.1

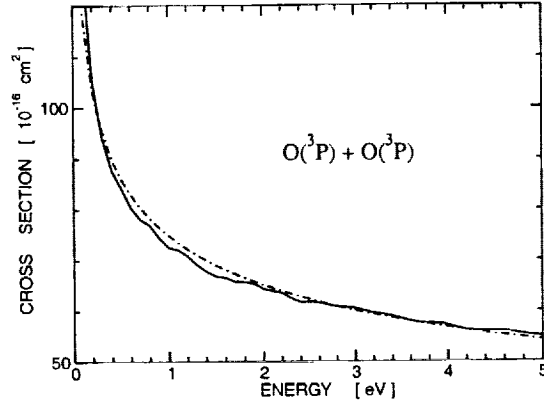


Fig.2

Total and differential cross sections were calculated for all individual spin states, and results have been statistically averaged over all spins. The calculated statistical cross sections (solid curve) are well described by the Landau-Schiff approximation (dashed curve) as shown in Fig.2 [Landau and Lifshitz, 1991]. The computed differential cross sections of O + O collisions are given in Fig.3 as functions of the scattering angle for collision energies of 0.03 , 0.3 and 3 eV.

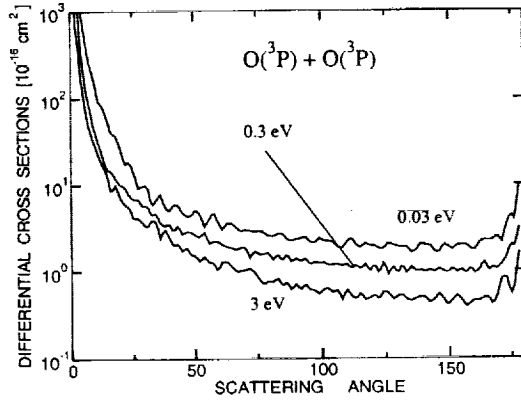


Fig.3

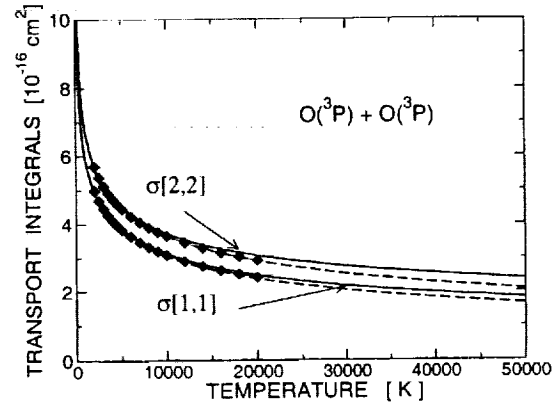


Fig.4

Strong angular anisotropy of differential cross sections is induced by long-range van der Waals forces. The statistically averaged cross sections are similar to those for elastic collisions of excited oxygen atoms [Yee and Dalgarno 1985, 1987].

New values of the transport coefficients in oxygen gas

Transport properties of the hot nitrogen and hydrogen atoms in the terrestrial atmosphere were calculated using accurate differential cross sections of elastic and inelastic collisions. Collisions of energetic oxygen and nitrogen atoms with thermal atomic oxygen are most important for the altitudes above 180 km. The reduced transport integrals, which are widely used for the simplified description of momentum and energy relaxation processes [Chapman and Cowling 1970], were calculated as functions of the gas temperature and were compared with previous theoretical and experimental data. In Fig.4 results of our calculations of the $\sigma[1, 1]$ and $\sigma[2, 2]$ transport integrals in $O(^3P) + O(^3P)$ collisions are shown by solid curves, the dashed curves show the results of quasi-classical calculations by Levin *et al.* (1990), and the diamonds are the results of classical trajectory calculations by Holland and Biolsi (1988).

The self-diffusion coefficient D_s and the viscosity η [Chapman and Cowling 1970; Ferziger and Kaper 1972] have been calculated for the temperature interval of 100 K - 30000 K and have been compared with available data [Dalgarno and Smith 1962; Levin *et al.* 1990]. Calculated transport coefficients D_s and η may be fitted by interpolation formulas

$$D_s \simeq \frac{10^{17}}{n_0} * T^{0.8} \text{ cm}^2 \text{ s}^{-1}, \quad \eta \simeq 2.72 * T^{0.76} * 10^{-6} \text{ g cm}^{-1} \text{ s}^{-1},$$

where T and n_0 are the temperature and the density of the atmospheric oxygen gas.

Energy relaxation of hot O and N atoms in the terrestrial thermosphere

Accurate differential cross sections of O and N collisions with atmospheric atoms and molecules have been used in evaluations of the energy relaxation kernel $B(E_f|E_i)$, which gives the rate of transitions from the state with initial energy E_i to the final state with translational energy E_f [Oppenheim *et al.* 1977]. The collision kernel has been calculated using analytical and numerical methods, developed in our investigations of the thermalization of hot nitrogen and oxygen atoms [Kharchenko *et al.* 1997, 1998, 2000; Balakrishnan *et al.* 1998a, 1999, 2000]. In Fig.5 the calculated rates of $E_i \rightarrow E_f$ transitions at different initial energies of 0.1, 1, 2.5 and 4.5 eV are shown for oxygen atoms thermalizing in the oxygen gas with the temperature of 850 K and the density of $3 \cdot 10^9 \text{ cm}^{-3}$ [Kharchenko *et al.* 2000]. The energy transition rate for the atmospheric gas mixture is calculated as a statistically weighted sum of the collisional kernels $B_i(E_f|E_i)$ of the individual atmospheric gases ($i = O, N_2$, and O_2). The rate of energy transitions $B(E_f|E_i)$ strongly depends on the altitude, because of the altitude dependence of the gas

density and composition. We have calculated the energy-transfer rates for fast oxygen atoms in the terrestrial atmosphere between 100 and 600 km. The rate of atmospheric heating normalized to a single hot O atom with given initial energy E has been also computed at different altitudes. Results are shown in Fig.6 as function of kinetic energy E for the altitude range from 100 km to 400 km.

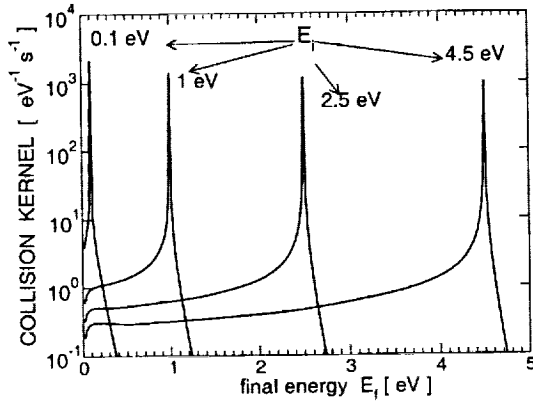


Fig.5

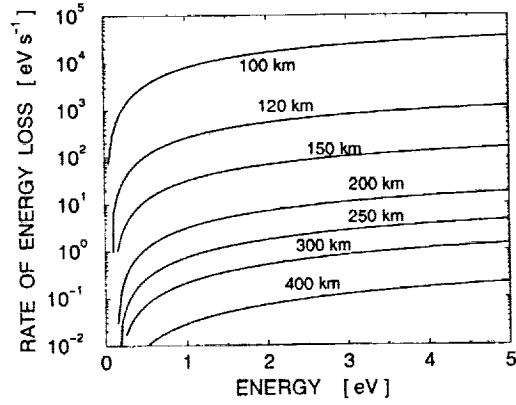


Fig.6

Times of thermalization of fast atoms depend on their initial energies. Distribution of the kinetic energies of nascent fast atoms produced by the various photo-chemical and ionic reactions [Richards *et al.* 1994; Hickey *et al.* 1995; Fox and Hac 1997] are shown in Fig.7 by dashed curves at 200, 300, and 400 km. In the same figure, the thermalization times of energetic O atoms at different altitudes were calculated with accurate quantal cross sections [Kharchenko *et al.* 2000].

We calculated the numbers of collisions, which are required for the thermalization of energetic O and N atoms in the atmospheric gas at different altitudes. The number of thermalizing collisions increases dramatically, if the initial energy of the nascent hot atom increases. Because of the strong anisotropy of differential cross sections the hot atoms lose their energy mostly by small amounts in long distance collisions with ambient atoms and molecules.

Energy relaxation process involves dozens of collisions, and the thermalization time increases significantly with the altitude. In Fig.7 the thermalization times for the atoms with different initial energies E [eV] are shown by solid lines for altitudes 200-400 km. Thermalization times of O and N atoms and rates of their energy losses were calculated for daytime and nighttime conditions of the terrestrial thermosphere. Rates of energy losses of fast $O(^3P)$ and $N(^4S)$ in collisions with atmospheric atoms and molecules were calculated for gas temperatures, densities, and compositions corresponding to the parameters of the terrestrial thermosphere between 100 - 600 km.

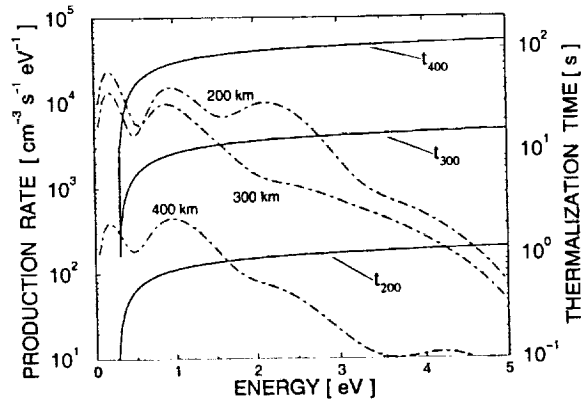


Fig.7

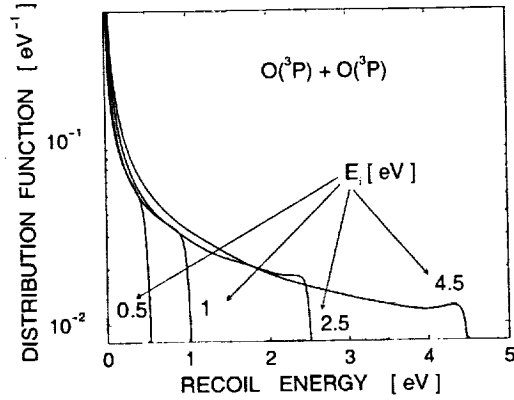


Fig.8

Secondary hot oxygen atoms in the upper thermosphere

In the middle and high regions of the terrestrial thermosphere, where atomic oxygen is the main constituent of the atmospheric gas, secondary hot $O(^3P)$ atoms arise in recoil collisions of nascent energetic atoms. Due to high efficiency of the energy transfer in $O-O$ collisions the recoil atoms may receive significant fraction of the kinetic energy, which was carried initially by nascent fast atoms. Recoil oxygen atoms play an important role in the formation of upward fluxes of energetic O atoms. We calculated the energy distribution of the secondary energetic oxygen atoms in binary collisions with fast N and O . These data have been used in our evaluations of the kinetics of hot atoms and in computing of atomic upward fluxes near the exobase.

Energy spectra of the resulting secondary energetic atoms have been obtained in quantum mechanical calculations of the energy transfer in $O + O$ collisions [Kharchenko *et al.* 200]. In Fig.8 the spectra of recoil oxygen atoms computed with accurate energy-transfer cross sections of $O + O$ collisions are shown for different initial energies E_i of nascent hot O atoms. Distribution functions of recoil atoms are normalized to unity. Number of recoil atoms increases exponentially with time, but their spectra converge asymptotically to the thermal distribution.

Non-Maxwellian distributions of fast O and N atoms

Calculations of non-Maxwellian distribution functions of fast O and N atoms are based on the solution of the Boltzmann equation describing the thermalization of the nascent energetic atoms [Shizgal and Blackmore 1986; Shizgal 1987; Stamnes *et al.* 1991; Lie-Svendsen *et al.* 1991, 1992; Shematovich *et al.* 1992, 1994, 1999; Bisikalo *et*

al. 1995; *Sharma et al.* 1996 ; *Gerard et al.* 1995, 1997; *Kharchenko et al.* 1997, 1998, 2000; *Balakrishnan et al.* 1998a,b, 1999, 2000; *Hubert et al.* 1999; *Kharchenko and Dalgarno* 2000a,b]. Solutions of the Boltzmann equation or Monte Carlo simulations of the energy relaxation process provide accurate non-Maxwellian distribution functions and escape fluxes of energetic atoms, if realistic differential cross sections of thermalizing collisions are used. Reported in the literature solutions of the kinetic equation and Monte Carlo simulations were mostly carried out for the hard sphere model, which assumes collisional cross sections independent of the energy and scattering angles [*Shizgal and Blackmore* 1986; *Shizgal* 1987; *Stamnes et al.* 1991; *Lie-Svendsen et al.* 1991, 1992; *Shematovich et al.* 1992, 1994, 1999; *Sharma et al.* 1996; *Marov et al.* 1997; *Hubert et al.* 1999]. With this model the calculation procedure is simplified significantly. However, the hard sphere approximation does not describe adequately the energy-transfer collisions, because realistic cross sections of atom-atom and atom-molecule collisions are strongly focused in the forward direction and depend on the collision energy [*Kozyra et al.* 1982; *Yee and Dalgarno* 1985, 1987; *Gerard et al.* 1997; *Kharchenko et al.* 1997, 1998, 2000; *Balakrishnan et al.* 1998a,b, 1999, 2000].

The new approach, which incorporates the quantum treatment of elastic and inelastic collisions with the solution of the Boltzmann equations, was developed for calculations of the energy distribution function of fast nitrogen atoms in the terrestrial thermosphere [*Kharchenko et al.* 1997, 1998; *Balakrishnan et al.* 1998a, 2000]. Recently it has been used to compute the energy relaxation of the ground-state and excited O and N atoms in the atmosphere [*Balakrishnan et al.* 1998b, 1999; *Zygelman et al.* 1999; *Kharchenko et al.* 2000; *Balakrishnan et al.* 2000; *Kharchenko and Dalgarno* 2000b].

The kinetic equations for thermalization of fast O and N atoms

Thermalization of hot atoms in the terrestrial thermosphere is governed by elastic and inelastic collisions with the thermal $O(^3P)$ atoms and N_2 and O_2 molecules. The computing scheme for calculations of the energy relaxation and the upward fluxes of fast O and N atoms are complicated by the presence of nascent metastable O and N atoms. Quenching collisions of excited atoms with atmospheric gas generate fast ground state O and N atoms, and distributions of ground state and excited atoms should be calculated self-consistently. Solutions of the Boltzmann equations allow to calculate upward fluxes of metastable and ground states atoms in consistent conditions. From the steady state solutions the altitude profiles and energy distributions of thermospheric oxygen and nitrogen were determined and compared with available observations and theoretical predictions [*Cotton et al.* 1993; *Gerard et al.* 1995, 1997; *Oliver* 1997; *Swaminathan et al.* 1998; *Hubert et al.* 1999; *Oliver and Schoendorf* 1999; *Litvin et al.* 2000; *Kharchenko et al.* 2000; *Kharchenko and Dalgarno* 2000b, 2001; *Balakrishnan et al.* 2000; *Schoendorf et al.* 2000].

Collisions between fast particles may be neglected in investigations of upward fluxes of energetic atoms, because hot atoms are only a minor fraction below 700-800 km [Cotton et al. 1993; Bisikalo et al. 1995; Gerard et al. 1995; Shematovich et al. 1999; Kharchenko and Dalgarno 2000b, 2001]. At higher altitudes atomic fluxes are well described by collisionless transport. The system of the Boltzmann equations for the momentum distribution functions $F_i(\vec{p}, z, t)$ of hot atoms with the identities of $i = \{O(^3P), O(^1D), O(^1S), N(^4S), N(^2D)\}$ are given by

$$\frac{\partial}{\partial t} F_i(\vec{p}, z, t) + m_i \vec{g} * \nabla_{\vec{p}} F_i(\vec{p}, z, t) + \frac{p_z}{m} \frac{\partial}{\partial z} F_i(\vec{p}, z, t) = \int d\vec{p}_1 F_i(\vec{p}_1, z, t) W_i(\vec{p}, \vec{p}_1, n_z) - \omega_i(p, z) F_i(\vec{p}, z, t) + Q_i(\vec{p}, z, t),$$

where m_i is the mass of the fast atom, \vec{g} is the free-fall acceleration, z is the vertical axes, $Q_i(\vec{p}, z, t)$ is the intensity of the source reactions, $\omega_i(\vec{p}, z)$ is the frequency of elastic and inelastic collisions between fast atoms and the ambient thermal gas, and $W_i(\vec{p}, \vec{p}_1, n_z)$ is the momentum relaxation rate depending on the differential cross sections of elastic and inelastic collisions and on the composition, temperature and density $n_z = n(z)$ of the atmospheric gas. The collisions, describing quenching of metastable O and N atoms, are taken into account in the source functions of fast $O(^3P)$ and $N(^4S)$ atoms [Gerard et al. 1995; Hickey et al. 1995; Shematovich et al. 1999; Kharchenko and Dalgarno 2000b]. In the upper thermosphere, secondary energetic recoil $O(^3P)$ atoms are included in the source function with the spectra shown in Fig.8 [Zygelman et al. 1999; Kharchenko et al. 2000]. Analytical expressions of the collision kernel via differential and doubly differential cross sections of elastic and inelastic collisions, which have been used in our numerical computations, were reported in articles [Kharchenko et al. 1997, 1998; Balakrishnan et al. 1998a,b; Shizgal 1999].

An alternative method for the numerical solution of the kinetic equation involves Monte Carlo simulations of multiple collisions between energetic atoms and the thermal atmospheric gas [Shematovich et al. 1994, 1999; Bisikalo et al. 1995; Gerard et al. 1995; Hubert et al. 1999; Kharchenko and Dalgarno 2001].

Monte Carlo simulations of upward traveling fluxes

Monte Carlo simulations may be a very efficient method of calculations of upward fluxes of fast atoms, once accurate energy and angular dependences of scattering cross sections have been used for the description of stochastic binary collisions. Monte Carlo simulations were carried out in our recent calculations to determine the energy and angular distributions in the vertical flux of hot $O(^3P)$ atoms [Kharchenko and Dalgarno 2001].

- An ensemble of hot oxygen atoms with energies E_{in} has been generated at different

initial altitudes H_{in} . Initial velocity directions of nascent fast atoms have been given by random numbers, and initial energy distributions have been compiled from the known spectra of source reactions.

- Collisions of ground state hot atoms with the thermal gas were described by four stochastic variables: j - the index of the identity of the bath gas atoms or molecules (O or N₂ for the atmosphere above 200 km); \vec{R} - the projectile radius-vector with the altitude projection of z ; θ - the angle between the velocity \vec{V} and the vertical axes z ; χ - the Center of the Mass Frame (CMF) scattering angle ($0 \leq \chi \leq \pi$); Φ - the azimuthal angle between the scattering and $[\vec{V}, \vec{e}_z]$ planes ($0 < \Phi < 2\pi$).
- The altitude, angular, and energy distributions of hot oxygen atoms have been obtained from the results of Monte Carlo simulations of multiple collisions between fast atoms and atoms of the ambient gas.

These distributions have been used to compute the fractions of energetic atoms escaping from the thermosphere to the exosphere [Lie-Svendsen et al. 1992; Hubert et al. 1999; Kharchenko and Dalgarno 2001]. In Fig.9 the calculated probabilities to escape into the exosphere (above 700 km) are shown as function of the initial altitude, where nascent fast O(³P) atoms have been produced. For atoms with the initial energy of 5 eV initial altitudes have been taken from 400 km to 700 km.

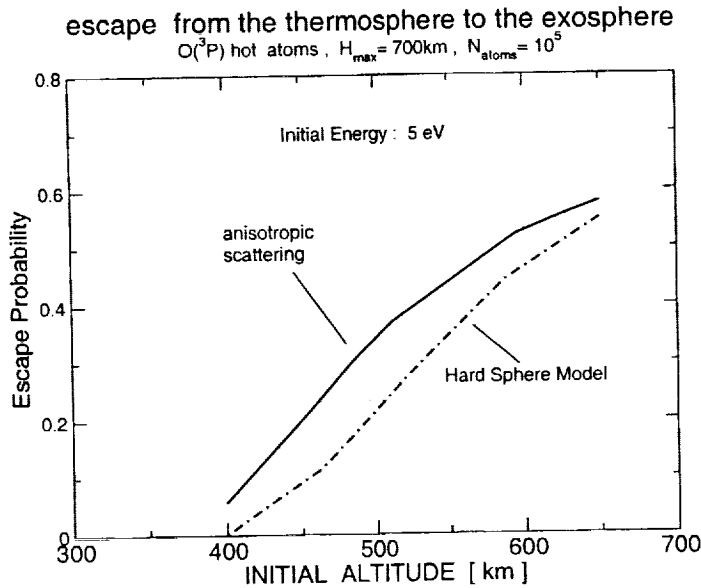


Fig.9

Calculations have been carried out for the quantally computed anisotropic cross sections and for the hard sphere model. Monte Carlo simulations have been used for computing upward fluxes of energetic O and N atoms in the upper thermosphere.

Time-dependent calculations of the energy relaxation.

The time-dependent energy distributions of nascent hot atoms provide detailed information on the relaxation rate and local heating of the ambient gas in conditions of variable sources of fast atoms. Time-dependent thermalization of energetic O and N atoms in the exobase region have been studied at variable magnetospheric and ionospheric conditions, and at different levels of solar activity. For the solution of the time-dependent Boltzmann equation we developed an efficient numerical method based on the matrix representation of the evolution operator via the energy relaxation kernel [Zygelman *et al.* 1999; Kharchenko and Dalgarno 2000b, 2001]. The results of our investigations of the energy relaxation of metastable and ground state O atoms and ground state N atoms have been reported recently [Balakrishnan *et al.* 1999; Zygelman *et al.* 1999; Kharchenko and Dalgarno 2000a,b], and the theoretical data have been compared with the results of laboratory measurements [Matsumi *et al.* 1994; Matsumi and Chowdhury 1996; Balakrishnan *et al.* 1999; Caledonia 2000]. Numerical solutions of the kinetic equation with realistic differential cross sections provide reliable information on the energy relaxation. In Fig.10 the results of our calculations of the energy loss of $O(^1D)$ atoms in the N_2 atmosphere are shown to be in excellent agreement with the experimental data [Matsumi *et al.* 1994; Matsumi and Chowdhury 1996; Balakrishnan *et al.* 1999].

Time-dependent solutions of the Boltzmann equation have been used for investigations of the time evolution of energy distributions of $O(^3P)$ and $N(^4S)$ atoms in the terrestrial thermosphere [Zygelman *et al.* 1999; Kharchenko *et al.* 2000; Kharchenko and Dalgarno, 2000a,b]. Fig.11 shows the time-dependent energy distributions of energetic oxygen atoms in the terrestrial thermosphere at 0.03 s, 0.17 s, 0.34 s and 1.35 s after they have been produced. All distributions are normalized to unity.

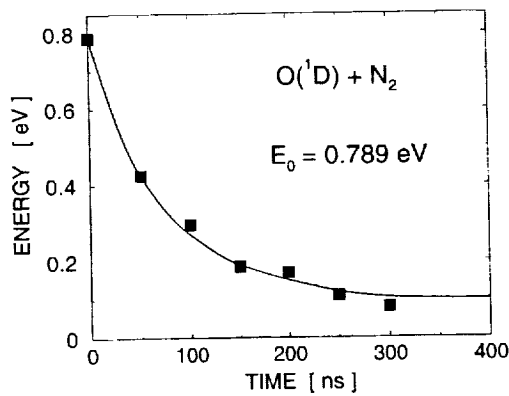


Fig.10

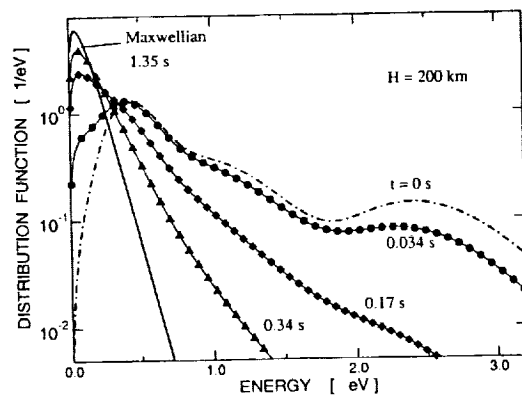


Fig.11

We included in our calculations more than twenty sources of nascent hot oxygen atoms [Shematovich *et al.* 1994; Gerard *et al.* 1995; Hickey *et al.* 1995].

Computational method, which has been developed in the present proposal, could be used in calculations of energy distributions of metastable and excited atoms. The energy and velocity relaxation of nascent metastable atoms may be determined from solutions of the time-dependent Boltzmann equations, and resulting distributions could be used in calculations of the Doppler profiles of $O(^1D, ^1S)$ emissions detected in the atmospheric observations [Schmitt *et al.* 1981, 1982; Killeen and Hayes 1981, 1983, 1984; Shematovich *et al.* 1999].

References

Balakrishnan, N., V. Kharchenko, and A. Dalgarno, Quantum mechanical and semi-classical studies of $N + N_2$ collisions and their application to the thermalization of fast N atoms, *J. Chem. Phys.*, **108**, 943, 1998a.

Balakrishnan, N., V. Kharchenko, and A. Dalgarno, Slowing of energetic $O(^3P)$ atoms in collisions with N_2 , *J. Geophys. Res.*, **103**, 23393, 1998b.

Balakrishnan, N., V. Kharchenko, and A. Dalgarno, Translational energy relaxation of hot $O(^1D)$ atoms, *J. Phys. Chem.*, **103**, 3999, 1999.

Balakrishnan N., E. Sergueeva, V. Kharchenko, and A. Dalgarno, Kinetics and thermalization of hot $N(^4S)$ atoms in the upper atmosphere, *J. Geophys. Res.*, **105**, 18549, 2000.

Bisikalo, D.V., V.I. Shematovich, J.-C. Gerard, A kinetic model of the formation of the hot oxygen geocorona. 2. Influence of O^+ ion precipitation, *J. Geophys. Res.*, **100**, 3715, 1995.

Caledonia G. E., Infrared Radiation Produced in Ambient/Spacecraft-Emitted gas interactions under LEO conditions, 38th *AIAA Aerospace Sciences Meeting*, Reno, Nevada, 2000.

Chapman, S., T. G. Cowling, *The mathematical theory of non-uniform gases*, Third edition, Cambridge, 1970.

Cotton, D. M., G. R. Gladstone, and S. Chakrabarti, Sounding rocket observation of a hot atomic oxygen geocorona, *J. Geophys. Res.*, **98**, 21651, 1993.

Dalgarno A. and F. J. Smith, The thermal conductivity and viscosity of atomic oxygen, *Planet. Space Sci.*, **9**, 1, 1962.

Ferziger, J. H., H. G. Kaper, *Mathematical theory of transport process in gases*, Elsevier Inc., New York, 1972.

Fox, J. L. and A. Hać, Spectrum of hot O at the exobase of the terrestrial planets, *J. Geophys. Res.*, **102**, 24005 (1997)

Gerard, J.-C., P. G. Richards, V. I. Shematovich and D. V. Bisikalo, The importance of new chemical sources for the hot oxygen geocorona, *Geophys. Res. Lett.*, **22**, 279,

1995.

Gerard J. C., D. V. Bisikalo, V. I. Shematovich and J. W. Duff, An updated model of the hot nitrogen atom kinetics and thermospheric nitric oxide, *J. Geophys. Res.*, **102**, 285, 1997.

Hickey M. P., Richards, and D. G. Torr, New sources for the hot oxygen geocorona: solar cycle, seasonal, latitudinal, and diurnal variations, *J. Geophys. Res.*, **100**, 17377, 1995.

Holland, P. M., L. Biolsi, Transport properties of ground state oxygen atoms, *J. Chem. Phys.*, **85**, 3203, 1988.

Hubert B., J.-C. Gerard, D. M. Cotton, D. V. Bisikalo and V. Shematovich, Effect of hot oxygen on thermospheric OI UV airglow, *J. Geophys. Res.*, **104**, 17139, 1999.

Kharchenko V., J. Tharamel and A. Dalgarno, Kinetics of thermalization of fast nitrogen atoms beyond the hard sphere approximation, *J. Atmos. Sol.-Ter. Phys.*, **59**, 107, 1997.

Kharchenko V., N. Balakrishnan, and A. Dalgarno, Thermalization of fast nitrogen atoms in elastic and inelastic collisions with molecules of atmospheric gases, *J. Atmos. Sol.-Ter. Phys.*, **60**, 95, 1998.

Kharchenko V., A. Dalgarno, B. Zygelman, and J.-H. Yee, Energy transfer in collisions of oxygen atoms in the terrestrial atmosphere, *J. Geophys. Res.*, **105**, 24899, 2000.

Kharchenko V., and A. Dalgarno, The upward flux of fast oxygen atoms in the terrestrial thermosphere, *Eos. Trans. AGU*, **81**, S333, 2000a.

Kharchenko V., and A. Dalgarno, Fraction of energetic oxygen atoms in the upper terrestrial thermosphere, *Eos Trans. AGU*, **81**, F931, 2000b.

Kharchenko V. and A. Dalgarno, Fluxes of fast atoms near the terrestrial thermosphere, *Eos. Trans. AGU*, **82**, S293, 2001.

Killeen, T.L. and P.B. Hays, Nonthermal line profiles from O(1S) in the thermospheric nightglow, *Appl. Optics*, **20**, 3314, 1981.

Killeen, T.L. and P.B. Hays, O(1S) from dissociative recombination of O₂⁺: non-thermal line profile measurements from Dynamics Explorer, *J. Geophys. Res.*, **88**, 10163, 1983.

Killeen, T.L. and P.B. Hays, Doppler line profile analysis for a multichannel Fabry-Perot interferometer, *Appl. Optics*, **23**, 619, 1984.

Kozyra J. U., T. E. Cravens, and A. F. Nagy, Energetic O⁺ Precipitation, *J. Geophys. Res.*, **87**, 2481, 1982.

Landau, L. D., and E. M. Lifshitz, *Quantum Mechanics*, Pergamon Press, Oxford, 1991.

Levin, E., H. Partridge, and J. R. Stallcop, Collision Integrals and High temperature Transport properties of N - N, O - O and N - O, *J. Thermophys.*, **4**, 496, 1990.

Lie-Svendsen, O., M. H. Rees, K. Stamnes and E. C. Whipple, The kinetics of hot nitrogen atoms in upper atmospheric neutral chemistry, *Planet. Space Sci.*, **39**, 929,

1991.

Lie-Svendsen, O., M. H. Rees and K. Stamnes, Helium escape from the Earth's atmosphere: the charge exchange mechanism revisited, *Planet. Space Sci.*, **40**, 1639, 1992.

Litvin, A. V., W. L. Oliver, Hot O and nighttime ionospheric temperatures at Saint Santin from 1968 to 1981, *EOS AGU*, **81**, S332, 2000.

Marov, M., V. I. Schematovich, D. V. Bisikalo, and J. C. Gerard, *Non-equilibrium processes in the planetary and cometary atmospheres: theory and applications*, Kluwer Academic Publishers, Boston, 1997.

Matsumi Y., M. Shamsuddin, Y. Sato, M. Kawasaki, Velocity relaxation of hot $O(^1D)$ atoms in collisions with rare gases, N_2 and O_2 , *J. Chem. Phys.*, **101**, 9610, 1994.

Matsumi Y. and A. M. S. Chowdhury, Translational relaxation and electronic quenching of hot $O(^1D)$ by collisions with N_2 , *J. Chem. Phys.*, **104**, 7036, 1996.

Oliver, W. L., Hot oxygen and the ion energy budget, *J. Geophys. Res.*, **102**, 2503, 1997.

Oliver, W. L., and J. Schoendorf, Variations of hot O in the thermosphere, *Geophys. Res. Lett.*, **26**, 2829, 1999.

Oppenheim, I., K. E. Shuler, and G. H. Weiss, *Stochastic processes in chemical physics: the master equation*, The MIT Press, Cambridge, 1977.

Richards, P. G., M. P. Hickey, and D. G. Torr, New sources of the hot oxygen geocorona, *Geophys. Res. Lett.*, **21**, 657, 1994.

Schoendorf, J., L. A. Young, and W. L. Oliver, Hot oxygen profiles for incoherent scatter radar analysis of ion energy balance, *J. Geophys. Res.*, **105**, 12832, 2000.

Sharma, R. D., V. A. Kharchenko, Y. Sun and A. Dalgarno, Energy distribution of fast nitrogen atoms in the nighttime terrestrial thermosphere, *J. Geophys. Res.*, **101**, 275, 1996.

Schematovich, V. I., D. V. Bisikalo and J.-C. Gerard, The thermospheric odd nitrogen photochemistry: Role of nonthermal $N(^4S)$ atoms, *Ann. Geophys.*, **10**, 792, 1992.

Schematovich, V. I., D. V. Bisikalo and J.-C. Gerard, A kinetic model of formation of the hot oxygen geocorona. 1. Quiet geomagnetic conditions, *J. Geophys. Res.*, **99**, 217, 1994.

Schematovich, V., J.-C. Gerard, D. V. Bisikalo, and B. Hubert, Thermalization of $O(^1D)$ atoms in the thermosphere, *J. Geophys. Res.*, **104**, 4287, 1999.

Shizgal, R. and R. Blackmore, A collisional kinetic theory of a plane parallel evaporating planetary atmosphere, *Planet. Space Sci.*, **34**, 279, 1986.

Shizgal, B., Hot hydrogen and deuterium in the exosphere of Venus, *Adv. Space Res.*, **7**, 73, 1987.

Shizgal, B.D., Escape of H and D from Mars and Venus by energization with hot oxygen, *J. Geophys. Res.*, **104**, 14833, 1999.

Schmitt, G.A., V.J. Abreu, and P.B. Hays, Non-thermal $O(^1D)$ produced by dissociative recombination of O^{2+} : a theoretical model and observational results, *Planet.*

Space Sci., **29**, 1095, 1981.

Schmitt, G.A., V.J. Abreu, and P.B. Hays, Line shape of the non-thermal 6300 Å O(¹D) emission, *Planet. Space Sci.*, **30**, 457, 1982.

Stamnes, K., O. Lie-Svendsen and M. H. Rees, The linear Boltzmann equation in slab geometry: development and verification of reliable and efficient solution, *Planet. Space Sci.*, **39**, 1435, 1991.

Swaminathan P. K., D. F. Strobel, D. G. Kupperman, C. Krishna Kumar, L. Acton, R. DeMajistre, J.-H. Yee, L. Paxton, D. E. Anderson, D. J. Strickland, and J. W. Duff, Nitric oxide abundance in the mesosphere/low thermosphere region: roles of X rays, suprathermal N(⁴S) atoms and vertical transport, *J. Geophys. Res.*, **103**, 11579, 1998.

Yee J.-H., A. Dalgarno, Energy transfer of O(¹S) atoms in collision with O(³P) atoms, *Planet. Space Sci.*, **33**, 825, 1985.

Yee J.-H., A. Dalgarno, Energy transfer of O(¹D) atoms in collision with O(³P) atoms, *Planet. Space Sci.*, **35**, 399, 1987.

Zygelman B., A. Dalgarno, and R. D. Sharma, Molecular theory of collision-induced fine structure transitions in atomic oxygen, *Phys. Rev. A*, **49**, 2587, 1994a.

Zygelman B., A. Dalgarno, and R. D. Sharma, Excitation of the ³P fine structure levels of atomic oxygen in collisions with oxygen atoms, *Phys. Rev. A*, **50**, 3920, 1994b.

Zygelman B., V. Kharchenko, and A. Dalgarno, Thermalization of energetic oxygen atoms in the upper terrestrial thermosphere, *Eos. Trans. AGU*, **80**, F781, 1999.

